Enhanced selectivity in non-heme iron catalysed oxidation of alkanes with peracids

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Enhanced selectivity in non-heme iron catalysed oxidation of alkanes with peracids: evidence for involvement of Fe(IV)=O species.

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Supporting information

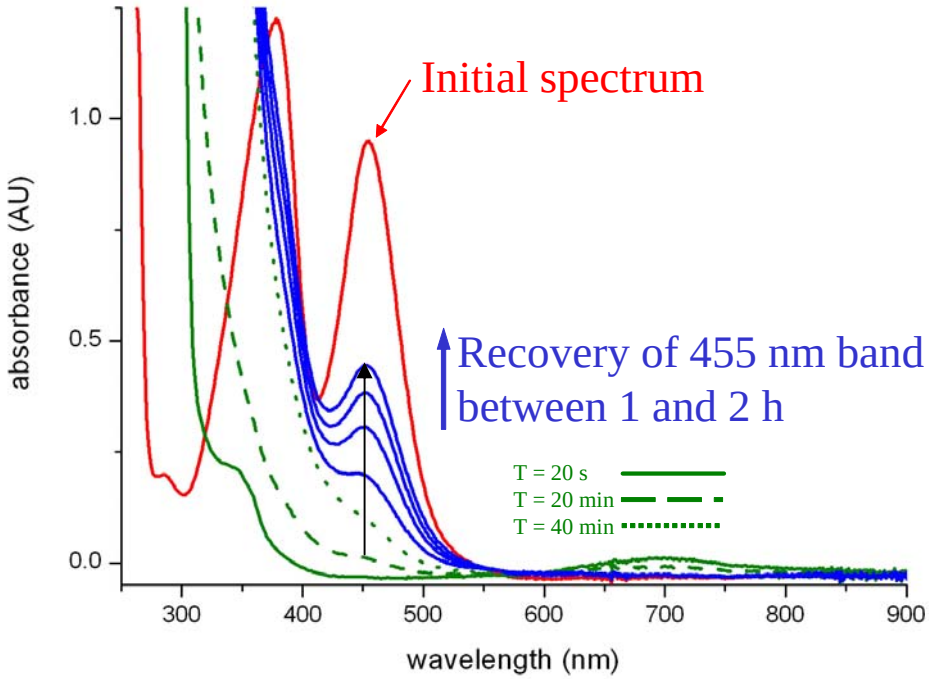

Figure S1 UV.Vis spectrum before (red), during (green) and after (blue) catalytic oxidation of cyclohexane in CH_3CN with *m*CPBA/**1a**, under N_2.

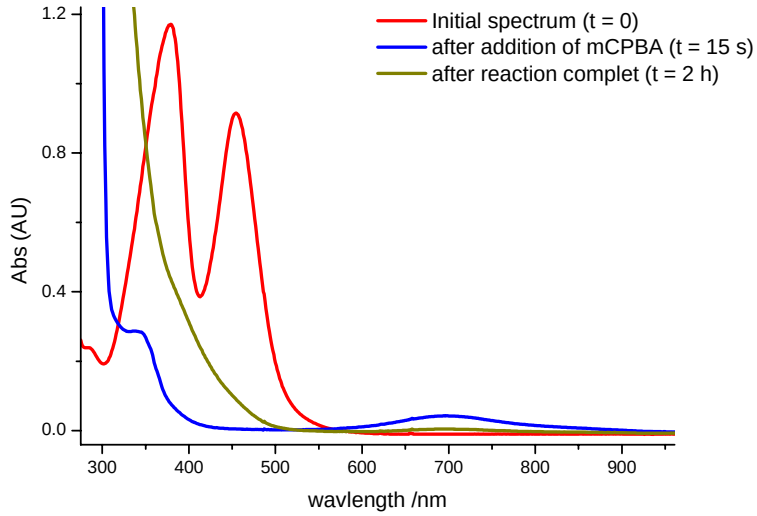

Figure S2 UV.Vis spectrum before (red), during (blue) and after (green) catalytic oxidation of cyclohexane in CH_3CN with *m*CPBA/**1a**, under O_2.

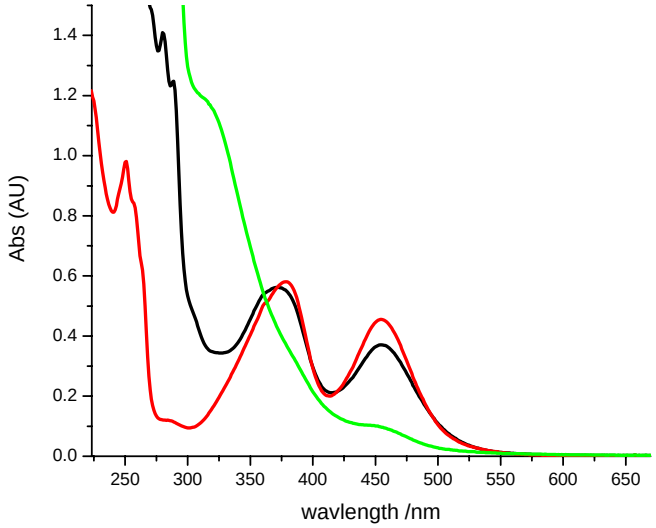

Figure S3 UV.Vis spectrum before (red) and 24 h after (reaction) catalytic oxidation of cyclohexane in CH_3CN with *m*CPBA/**1a**, under O_2 and after bulk reduction at -0.2 V vs SCE (see legend figure S4) (black).

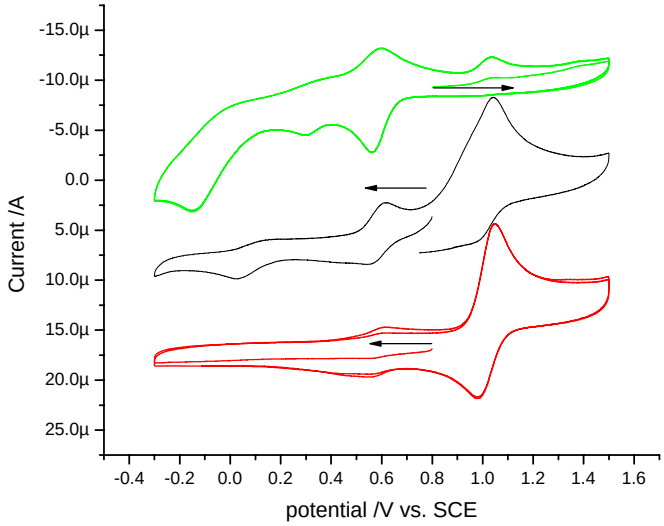

Figure S4 Cyclic voltammogram before (red) and 24 h after reaction (green) catalytic oxidation of cyclohexane in CH_3CN with *m*CPBA/**1a**, under O_2 and after bulk reduction (black) at -0.2 V vs SCE (Working electrode Pt Gauze, Counter electrode Pt Wire, using CHinstruments CHI630B). Initial scanning point and direction indicated by black arrow.

Analytical Data.

1a and **1b** were prepared analogous to literature procedures. Spectroscopic data are consistant with the stuctures.[i] Anal. calcd. for **1a**, $C_{25}H_{30}B_2F_8FeN_5 \cdot H_2O$: C 45.77, H 4.00, N 12.81; found: C 45.95, H 3.88, N 12.57. Anal. calcd. for **1b** $C_{87}H_{45}B_2F_{48}FeN_5$ C 48.61, H 2.11, N 3.26; found: C 47.80, H 2.29, N 3.56.

i) M. Lubben, A. Meetsma, E. C. Wilkinson, B. L. Feringa, L. Que, Jr., *Angew. Chem. Int. Ed. Engl.*, 1995, **34**, 1512; G. Roelfes, V. Vrajimasu, K. Chen, R. Y. N. Ho, J.-U. Rohde, C. Zondervan, R. M. la Crois, E. P. Schudde, M. Lutz, A. L. Spek, R. Hage, B. L. Feringa, E. Münck, L. Que, Jr., *Inorg. Chem.*, 2003, **42**, 2639.